Tarek A Mohamed

List of Publications by Year
in descending order

61 papers	861 citations	516710 16 h-index	580821 25 g-index
61 all docs	61 docs citations	61 times ranked	704 citing authors

#	Article	IF	Citations
1	Keto-enol tautomerism, spectral (infrared, Raman and NMR) studies and Normal coordinate analysis of 4-Methyl-2-hydroxyquinoline using quantum mechanical calculations. Journal of Molecular Structure, 2022, 1252, 132137.	3.6	2
2	Synthesis, structural, photo-physical properties and DFT studies of some diarylheptanoids. Journal of Molecular Structure, 2022, 1264, 133254.	3.6	5
3	Molecular structure and mild steel/HCl corrosion inhibition of 4,5-Dicyanoimidazole: Vibrational, electrochemical and quantum mechanical calculations. Journal of Molecular Structure, 2021, 1230, 129647.	3.6	43
4	Novel PVA/Methoxytrimethylsilane elastic composite membranes: preparation, characterization and DFT computation. Journal of Molecular Structure, 2021, 1235, 130173.	3.6	10
5	<scp>2â€Hydroxyâ€5â€nitropyridine and 5â€nitroâ€2â€pyridone: Tautomerism, infrared, Raman, and NMR spectral interpretations, normal coordinate analysis, and DFT calculations</scp>. Journal of the Chinese Chemical Society, 2021, 68, 1863-1879.	1.4	5
6	Molecular structure, tautomer's, reactivity and inhibition studies on 6-Methyl-2-thiouracil for mild steel corrosion in aqueous HCl (1.00 M): Experimental and Theoretical Studies. Journal of Molecular Structure, 2021, 1244, 130927.	3.6	31
7	Synthetic routes and vibrational analysis of 5-(4-Chlorophenyl) -3H-pyrazol-3-one molecule: Raman, Infrared and DFT calculations. Journal of Molecular Structure, 2021, 1245, 131036.	3.6	2
8	Thiadiazole-2-Thiol-5-Thione and 2,5-Dimercapto-1,3,4-Thiadiazol Tautomerism, Conformational Stability, Vibrational Assignments, Inhibitor Efficiency and Quantum Chemical Calculations. Zeitschrift Fur Physikalische Chemie, 2020, 234, 415-440.	2.8	8
9	Structure/property relationship of polyvinyl alcohol/dimethoxydimethylsilane composite membrane: Experimental and theoretical studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117810.	3.9	22
10	Raman, DRIFT and ATR-IR spectra, corrosion inhibition, DFT and solid-state calculations of 4-amino-3-choloro-2,5,6-trifluoropyridine. Journal of Molecular Structure, 2020, 1207, 127837.	3.6	3
11	Raman, Infrared and NMR Spectroscopy: Advances in Structural, Conformational and Environmental Analysis. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 566-567.	1.1	2
12	Synthesis, Conformational Analysis, Infrared, Raman and UV-Visible Spectra of Novel Schiff Bases compiled with DFT Calculations. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 568-586.	1.1	3
13	Computational studies, NMR, Raman and infrared spectral analysis of centrosymmetric (2Z,4Z)-Hexa-2,4-dienedinitrile. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950011.	1.8	3
14	Raman, infrared and NMR spectra, vibrational assignments and quantum mechanical calculations of centrosymmetric 3,6-Dicholoro-1,2,4,5-tetrazine. Journal of Molecular Structure, 2019, 1178, 298-304.	3.6	1
15	XPS and IR studies of plasma polymers layer deposited from allylamine with addition of ammonia. Applied Surface Science, 2018, 458, 1006-1017.	6.1	24
16	Synthesis, characterization, computational studies and biological activities of Co(II), Ni(II) and Cu(II) complexes of 2-Amino-1,3,4-thiadiazole derivatives. Journal of Coordination Chemistry, 2018, 71, 2814-2830.	2.2	4
17	Raman and DRIFT spectra, vibrational assignments and quantum mechanical calculations of centrosymmetric meso -2,3-Dimercaptosuccinic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 183, 275-283.	3.9	7
18	Conformational stability, spectral analysis (infrared, Raman and NMR) and DFT calculations of 2-Amino-5-(ethylthio)-1,3,4-thiadiazole. Journal of Molecular Structure, 2017, 1130, 434-441.	3.6	13

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19	Computational (DFT and MP2) and spectral interpretations, normal coordinate analysis, force constants and barriers to internal rotations of Trimethylacetonitrile. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650034.	1.8	2
20	Raman and infrared spectra, normal coordinate analysis and ab initio calculations of 4-Amino-2-chloropyrimidine-5-carbonitrile. Journal of Molecular Structure, 2016, 1115, 85-93.	3.6	6
21	Infrared, Raman and NMR spectral analysis, vibrational assignments, normal coordinate analysis, and quantum mechanical calculations of 2-Amino-5-ethyl-1,3,4-thiadiazole. Journal of Molecular Structure, 2016, 1103, 70-81.	3.6	11
22	Raman, infrared and NMR spectral analysis, normal coordinate analysis and theoretical calculations of 5-(methylthio)-1,3,4-thiadiazole-2(3H)-thione and its thiol tautomer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 339-349.	3.9	16
23	Structure of Plasma Poly(Acrylic Acid): Influence of Pressure and Dielectric Properties. Plasma Chemistry and Plasma Processing, 2015, 35, 303-320.	2.4	20
24	Raman and infrared spectra, crystal structure and DFT calculations of novel N-benzyl-4-(3-benzylcarbamoyl-propyldisulfanyl)-butyramide: [C6H5CH2NHC(O)(CH2)4S]2. Research on Chemical Intermediates, 2015, 41, 4761-4784.	2.7	2
25	Synthesis, antimicrobial activity, structural and spectral characterization and DFT calculations of Co(II), Ni(II), Cu(II) and Pd(II) complexes of 4-amino-5-pyrimidinecarbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 417-427.	3.9	34
26	Tautomerism, Raman, infrared and ultravioletâ€“visible spectra, vibrational assignments, MP2 and B3LYP calculations of dienol 3,4-dihydroxypyridine, keto-enol 3-hydroxypyridin-4-one and keto-enol dimer. Journal of Molecular Structure, 2013, 1043, 52-67.	3.6	7
27	Analysis of UV and vibrational spectra (FT-IR and FT-Raman) of hexachlorocyclotriphosphazene based on normal coordinate analysis, MP2 and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 446-455.	3.9	9
28	Infrared and NMR spectra, tautomerism, vibrational assignment, normal coordinate analysis, and quantum mechanical calculations of 4-amino-5-pyrimidinecarbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 111, 277-289.	3.9	10
29	DFT Simulation and Vibrational Analysis of the IR and Raman Spectra of a CdSe Quantum Dot Capped by Methylamine and Trimethylphosphine Oxide Ligands. Journal of Physical Chemistry C, 2012, 116, 14674-14681.	3.1	52
30	Infrared, 1H and 13C NMR spectra, structural charcterization and DFT calculations of novel adenine-cyclodiphosp(V)azane derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 304-313.	3.9	5
31	Infrared, Raman and NMR spectra, conformational stability, normal coordinate analysis and B3LYP calculations of 5-amino-4-cyano-3-(methylthio)-1H-pyrazole-1-carbothioamide. Journal of Molecular Structure, 2011, 985, 277-291.	3.6	15
32	Vibrational assignments, normal coordinate analysis, B3LYP calculations and conformational analysis of methyl-5-amino-4-cyano-3-(methylthio)-1H-pyrazole-1-carbodithioate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1722-1730.	3.9	10
33	Infrared, Raman and temperature-dependent NMR spectra, vibrational assignments, normal coordinate analysis, and DFT calculations of benzoxazoline-2-thione. Vibrational Spectroscopy, 2010, 52, 128-136.	2.2	15
34	Conformational stability, r 0 structural parameters, barriers to internal rotation, ab initio calculations, and vibrational assignment for 2,2-difluoroethanol. Structural Chemistry, 2009, 20, 489-503.	2.0	9
35	Tautomerism, normal coordinate analysis, vibrational assignments, calculated IR, Raman and NMR spectra of adenine. Journal of Molecular Structure, 2009, 938, 263-276.	3.6	57
36	Conformational stability, barriers to internal rotation of 2-aminothiophenol (d0 and d3): A combined vibrational and theoretical approach. Computational and Theoretical Chemistry, 2008, 865, 14-24.	1.5	16

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37	Reinvestigation of benzothiazoline-2-thione and 2-mercaptobenzothiazole tautomers: Conformational stability, barriers to internal rotation and DFT calculations. Computational and Theoretical Chemistry, 2008, 868, 27-36.	1.5	31
38	Raman spectrum, quantum mechanical calculations and vibrational assignments of (95% Î±-TeO2/5%) Tj ETQq0 0 0 rgBT /Overlock 10 T 450-454.	3.9	10
39	Conformational stability, vibrational assignmenents, barriers to internal rotations and ab initio calculations of 2-aminophenol (d0 and d3). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 688-700.	3.9	16
40	Chelates and corrosion inhibition of newly synthesized Schiff bases derived from o-tolidine. Transition Metal Chemistry, 2007, 32, 461-467.	1.4	27
41	Structural characterization of tellurite glasses doped with transition metal oxides using Raman spectra and ab initio calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 106-115.	3.9	11
42	Raman spectrum, conformational stability, barriers to internal rotations and DFT calculations of 1,1,1-trifluoro-propane-2-thione with double-internal-symmetric rotor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 800-807.	3.9	5
43	Some periodic trends, molecular structure, normal coordinate analysis of 1,3,5-trioxane, -trithiane and -triselenane: computational and vibrational studies. Computational and Theoretical Chemistry, 2005, 713, 179-192.	1.5	16
44	Vibrational analysis, conformational stability, force constants, barriers to internal rotations, RHF, MP2 and DFT calculations oftrans,trans-2,4-hexadiene. Journal of Raman Spectroscopy, 2004, 35, 869-878.	2.5	14
45	Conformational Stability from Variable-Temperature Infrared Spectra of Krypton Solutions, Ab Initio Calculations, and roStructural Parameters of Chlorocyclopentane. Structural Chemistry, 2003, 14, 617-635.	2.0	16
46	Conformational stability from variable temperature infrared spectra of krypton solutions, ab initio calculations, and vibrational assignment of bromocyclopentane. Journal of Molecular Structure, 2003, 645, 89-107.	3.6	14
47	Spectra and structure of silicon containing compounds XXXV infrared and Raman spectra, vibrational assignment, conformational stability, and ab initio calculations of dichloromethyldimethyl silane. Journal of Molecular Structure, 2003, 649, 7-24.	3.6	4
48	Structural parameters, barriers to internal rotation, normal coordinate analysis and quantum mechanics calculations of 1,1,1-trimethyldisilane. Computational and Theoretical Chemistry, 2003, 635, 161-172.	1.5	10
49	Spectra and structure of silicon-containing compounds.. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2099-2114.	3.9	15
50	Spectra and structure of silicon containing compounds. Vibrational Spectroscopy, 2002, 30, 111-120.	2.2	27
51	Title is missing!. Structural Chemistry, 1999, 10, 333-348.	2.0	28
52	Raman and infrared spectra, conformational stability, normal coordinate analysis,ab initio calculations and vibrational assignment of 1-chloro-1-methylsilacyclobutane. Journal of Raman Spectroscopy, 1999, 30, 399-411.	2.5	8
53	Title is missing!. Structural Chemistry, 1998, 9, 255-264.	2.0	28
54	Infrared and raman spectra, conformational stability, normal coordinate analysis, ab initio calculations, and vibrational assignment of difluoroacetyl fluoride. Journal of Molecular Structure, 1998, 444, 165-182.	3.6	3

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55	Spectra and structure of silicon-containing compounds. XVIII-Raman and infrared spectra, conformational stability, vibrational assignment, barrier to internal rotation and ab initio calculations of ethyldichlorosilane. Journal of Raman Spectroscopy, 1994, 25, 159-174.	2.5	19
56	Spectra and structure of silicon-containing compounds. XVII. Vibrational and microwave spectra, molecular structure, barrier to internal rotation and ab initio calculations of methyltrichlorosilane. Spectrochimica Acta Part A: Molecular Spectroscopy, 1994, 50, 621-637.	0.1	10
57	Spectra and structure of silicon compounds. XVII Raman and infrared spectra and vibrational assignment for hexamethyldisilane and ab initio calculations for disilane and hexamethyldisilane. Spectrochimica Acta Part A: Molecular Spectroscopy, 1994, 50, 639-660.	0.1	18
58	Spectra and structure of silicon-containing compounds. XIX. Raman and infrared spectra, conformational stability, vibrational assignment, barrier to internal rotation, and ab initio calculations of ethyldifluorosilane. Journal of Molecular Structure, 1994, 319, 109-127.	3.6	14
59	Raman and infrared spectra, conformational stability, barriers to internal rotation, ab initio calculations and vibrational assignment for bromodifluoroacetyl chloride. Journal of Raman Spectroscopy, 1993, 24, 1-10.	2.5	9
60	Infrared and Raman spectra, conformational stability, barrier to internal rotation, and ab initio calculations of 1,1-dichloropropane. Journal of Molecular Structure, 1993, 299, 111-140.	3.6	19
61	Ab Initio Study of the Vibrational Signatures for the Covalent Functionalization of Graphene. Journal of Physical Chemistry C, 0, , 130917155202007.	3.1	5